Appendix A
Biota-to-Sediment Accumulation Factors and Remedial Action Objectives

Appendix A
Biological Sediment Accumulation Factor and Remedial Action Objective Uncertainty Analysis

Summary

Confidence limits for biological sediment accumulation factors (BSAF) and sediment remedial action objectives (RAO) were estimated using bootstrapping, a computer resampling method. BSAFs and RAOs were calculated for each of seven aquatic biota sampling areas and sitewide. Sitewide sediment RAOs ranged from 0.032 mg/kg for a mixed (76 percent bass, 24 percent carp) diet for subsistence anglers to 0.17 mg/kg for central tendency anglers on a mixed fish fillet diet. BSAFs and RAOs were based on 263 fish fillet samples and 621 surficial (top 2 inches) sediment samples. Upper and lower confidence limits for RAOs tended to differ by approximately a factor of 2, although it is thought that decisions based on either upper or lower confidence limits would result in similar remedial decisions. Note that Section 6 of this risk assessment presents RBC_{sed} values that are not to be confused with the RAOs presented here for discussion. The stochastic analysis presented in this appendix was not used in the calculation of the RBC_{sed} values of Section 6.

Introduction

BSAFs and RAOs were calculated for each of seven aquatic biota study areas (ABSA) at the Allied Paper, Inc./Portage Creek/Kalamazoo River Superfund Site. BSAFs were based on lipid normalized fish fillets and organic carbon normalized sediment concentration, and RAOs were designed to be protective of 1×10^{-5} cancer risk for central tendency, high-end sport, and subsistence anglers. Approximately 95% confidence limits were calculated for BSAFs and RAOs.

Because BSAFs and RAOs are ratios of random variables, no formulas are available for their exact sampling variances, so approximately 95% confidence limits were estimated using bootstrap resampling (Efron 1982). Additionally, to check the accuracy of bootstrap estimates, Taylor series approximation (Cochran 1977) was used to estimate confidence limits for the BSAF at Lake Allegan. The bootstrap estimates are nonparametric, while the Taylor approximation requires the assumption that the sampling distribution is approximately normally distributed. Confidence limits for sediment RAOs were estimated for each ABSA separately and for the entire site (i.e., a sitewide RAO) for diets composed of 100 percent carp or smallmouth bass, and a combined diet composed of 76 percent bass and 24 percent carp.

Bootstrap Sampling Method

Bootstrap estimation is a computer intensive resampling method for estimating sampling distributions and confidence limits of statistics for which the theoretical sampling distribution is not known. To estimate 95% confidence limits for the mean of n samples, one would repeatedly (1,000 to 10,000 times) select n records with replacement from the original data and calculate the mean of each bootstrap sample. The 97.5th and 2.5th percentiles of the bootstrap distribution are estimates of the 95% confidence limits.

The bootstrap algorithm described in Figure 1 was implemented in MATLAB© (The Mathworks 1998). To ensure that the random sampling algorithm was unbiased, the number of times each sample record was included in a bootstrap sample was counted and displayed in histograms. To demonstrate the correct algorithm performance, the resulting histogram is included for Lake Allegan (Figure 2). The bootstrap distributions of normalized mean fillet and sediment concentrations are displayed in Figure 3. The bootstrap distribution of the BSAF at Lake Allegan is summarized in a histogram of cumulative distribution plot in Figure 4. Confidence limits for sitewide and ABSA-specific BSAFs and RAOs are summarized in Tables 1 through 7.

Taylor Series Approximation

Define C_f and C_s to be normalized PCB concentration in fish fillets and sediment respectively. The biological sediment accumulation factor is given by:

$$BSAF = \overline{C}_f / \overline{C}_s$$

Defining $Var(\overline{C}_k) = S_k^2 / n_k$ for (k=f,s) to be the variance of each mean, the first order Taylor series approximation to the variance of the BSAF is

$$Var(BSAF) \cong (BSAF)^2 x \left\{ \frac{var(\overline{C}_f)}{\overline{C}_f^2} + \frac{var(Cs)}{\overline{C}_s^2} - 2x \frac{Cov(\overline{C}_f, \overline{C}_s)}{\overline{C}_f x \overline{C}_s} \right\}$$

For sufficiently large sample sizes, approximately (1-∀) 100 percent confidence limits are given by:

$$BSAF \pm z_{a/2} \sqrt{Var(BSAF)}$$

Confidence limits for the BSAF at Lake Allegan were approximated using the Taylor approximation for comparison with the bootstrap estimates.

Results

Comparison of Bootstrap and Taylor Estimates at Lake Allegan

The bootstrap algorithm was implemented as in Figure 1. It can be seen in Figure 2 that each record had approximately uniform probability of inclusion in each bootstrap sample. The bootstrap distribution of average normalized fish and sediment concentrations are displayed in Figure 3. The average lipid normalized fish concentrations are symmetrically distributed about a mean of 156 (mg-PCB / kg-lipid), while the distribution of the average normalized sediment concentration is somewhat skewed toward higher values.

The 10,000 bootstrap estimates of the BSAF at ABSA 9 ranged from 0.35 to 2.8 with an average of 0.99 and a median of 0.94. The bootstrap estimated lower and upper 95% confidence limits are 0.55 and 1.68 respectively. The Taylor expansion estimated lower and upper 95% confidence limits are 0.39 and 1.48 respectively. The Taylor expansion confidence limits are similar to the bootstrap confidence limits. This similarity provides an added level of scientific credibility that the bootstrap algorithm is performing properly. It should be noted that the Taylor expansion requires the assumption of a symmetric interval, while the bootstrap distribution is somewhat asymmetric with a longer upper-, than lower-tail. Because fewer assumptions are required to justify it, the bootstrap interval is preferred. Confidence intervals for BSAFs and RAOs for the remaining ABSAs are based on bootstrap estimation.

Bootstrap BSAF and RAO Estimates

Average BSAFs for smallmouth bass ranged from 0.21 at ABSA 6 (Otsego City Dam) to 2.6 at ABSA 8 (Trowbridge Dam; Table 1) while for carp, BSAFs ranged from 0.34 at ABSA 7 (Otsego Dam) to 3.8 at ABSA 8 (Table 2). Sitewide BSAFs are approximated by averaging the BSAFs across ABSAs and reported in the last row of Tables 1 and 2.

Sitewide RAOs were estimated for fish tissue concentrations of 0.042, 0.023, 0.021, and 0.008 mg/kg in smallmouth bass and carp respectively (Tables 3 and 4). Sediment RAOs were also calculated for a mixed diet of 76 percent bass and 24 percent carp. To be protective of central tendency anglers (0.042 mg/kg fish tissue concentration) with a mixed diet, a sediment RAO of 0.17 is estimated with 95% confidence interval of 0.12- to 0.25-mg/kg (Table 5). To be protective of subsistence anglers on a mixed diet, a sediment RAO ranging from 0.021 to 0.048 is estimated (Table 5). ABSA specific upper 95% confidence limits on RAOs for smallmouth bass ranged from 0.15mg/kg at Trowbridge Dam to 3.7 mg/kg at Otsego City Dam; however, all other upper confidence limits were less than 1.0 mg/kg for both carp and bass (Tables 6 and 7).

The sampling variance of BSAFs and RAOs was estimated using bootstrap resampling procedures. In general, upper and lower confidence limits for RAOs differed by a factor of 2; however, all sitewide RAOs for mixed diets were less than 0.25 with 95% confidence. Given the practical limits of remedial technologies, a factor of 2 variability in RAO estimates is adequate precision to make remedial decisions.

References

Cochran, W. G. 1977. *Sampling Techniques*. John Wiley and Sons, New York.

Efron, B. 1982. The Jackknife, the Bootstrap and Other Resampling Methods. *Society for Industrial and Applied Mathematics*, CBMS-NSF Monograph 38.

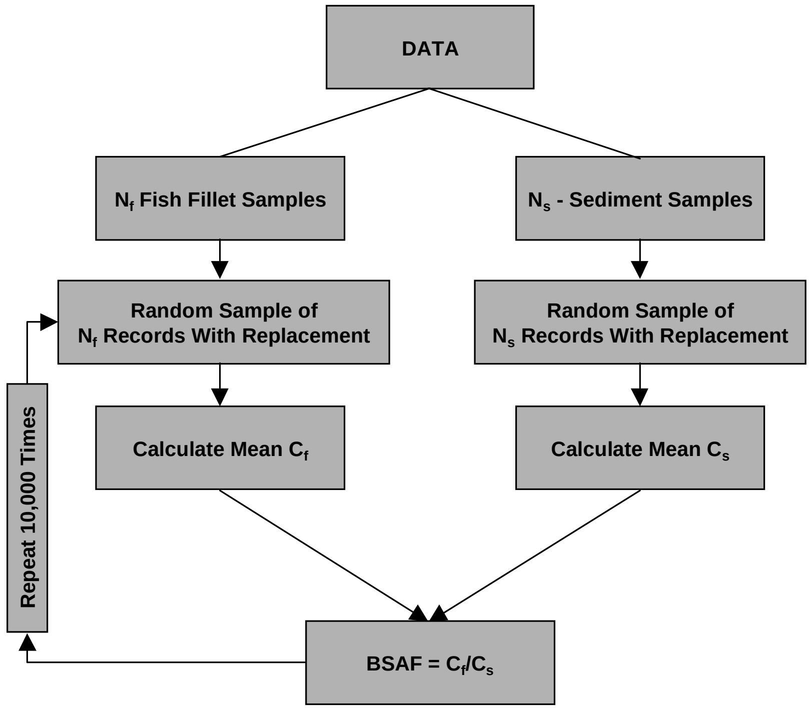

Figure 1 - Bootstrap sampling algorithm for the distribution of BSAF and RAO.

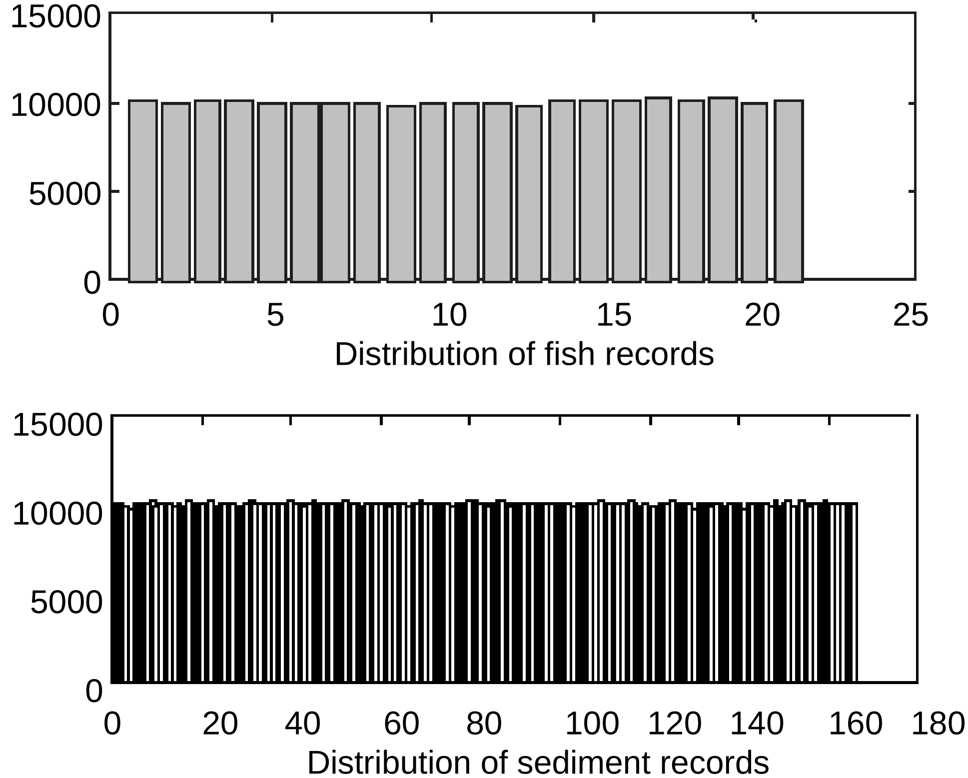

Figure 2 - Frequency of inclusion of each record among 10,000 bootstrap samples. There are 21 fish records and 166 sediment records.

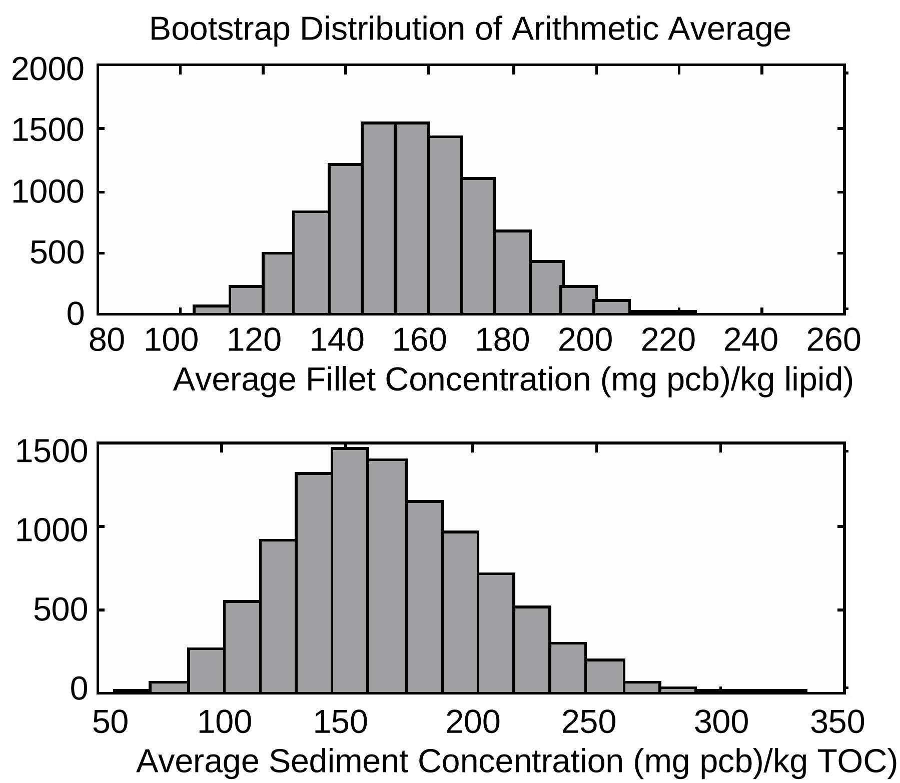

Figure 3 - Bootstrap distributions of arithmetic average normalized fillet and sediment concentrations ABSA 9.

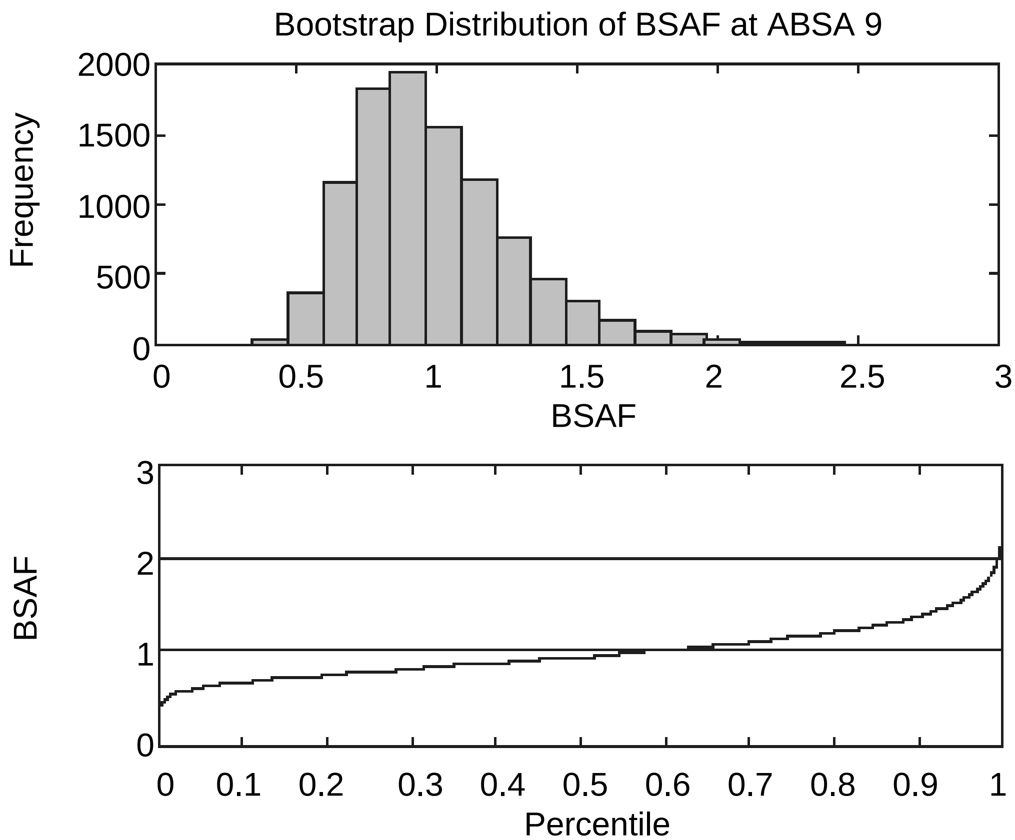

Figure 4 - Bootstrap distribution of BSAF at ABSA 9.

Table 1 Bootstrap Distributions of BSAF for Smallmouth Bass

ABSA	BSAF	Bootstrap BSAF Distribution			
		Mean	**Median**	**LCL95**	**UCL95**
3	0.296	0.314	0.301	0.182	0.515
4	0.604	0.669	0.620	0.343	1.261
5	0.432	0.638	0.443	0.194	1.916
6	0.092	0.208	0.099	0.028	0.891
7	0.371	0.470	0.393	0.183	1.161
8	2.296	2.590	2.373	1.303	5.148
9	0.708	0.755	0.723	0.438	1.249
Sitewide Average		0.806	0.707	0.382	1.735

Table 2 Bootstrap Distributions of BSAF for Common Carp

ABSA	BSAF	Bootstrap BSAF Distribution			
		Mean	**Median**	**LCL95**	**UCL95**
3	0.523	0.557	0.536	0.302	0.939
4	1.113	1.235	1.155	0.636	2.298
5	0.313	0.466	0.332	0.143	1.455
6	0.202	0.463	0.219	0.068	1.954
7	0.275	0.341	0.288	0.124	0.861
8	3.437	3.854	3.506	1.807	7.990
9	0.935	0.991	0.950	0.554	1.677
Sitewide Average		1.130	0.998	0.519	2.453

Table 3 Sitewide PCB Concentrations in Sediment Protective for Selected Levels of Smallmouth Bass Tissue Concentrations

Tissue (mg/kg)		Bootstrap RAO Distribution (mg/kg)			
		Mean	**Median**	**LCL95**	**UCL95**
0.042	0.203	0.205	0.200	0.136	0.300
0.023	0.111	0.112	0.109	0.073	0.163
0.021	0.101	0.102	0.099	0.066	0.150
0.008	0.039	0.039	0.038	0.026	0.058

Table 4 Sitewide PCB Concentrations in Sediment Protective for Selected Levels of Carp Tissue Concentrations

Tissue (mg/kg)		Bootstrap RAO Distribution (mg/kg)			
		Mean	**Median**	**LCL95**	**UCL95**
0.042	0.063	0.064	0.062	0.041	0.093
0.023	0.028	0.028	0.027	0.018	0.043
0.021	0.031	0.032	0.031	0.021	0.046
0.008	0.012	0.012	0.012	0.008	0.018

Table 5 Sitewide PCB Concentrations in Sediment Protective for 76 Percent Smallmouth Bass and 24 Percent Carp Tissue Concentrations

Tissue (mg/kg)	Bootstrap RAO Distribution (mg/kg)			
	Mean	Median	LCL95	UCL95
0.042	0.170	0.166	0.112	0.248
0.023	0.091	0.089	0.059	0.133
0.021	0.084	0.082	0.055	0.124
0.008	0.032	0.031	0.021	0.048

Table 6 PCB Concentrations in Sediment Protective for Selected Levels of Smallmouth Bass Tissue Concentrations

	Tissue (mg/kg)	Data RAO	Bootstrap RAO Distribution (mg/kg)			
			Mean	Median	LCL95	UCL95
3	0.042	0.119	0.122	0.115	0.059	0.225
4	0.042	0.167	0.171	0.163	0.077	0.311
5	0.042	0.416	0.410	0.390	0.096	0.854
6	0.042	1.196	1.289	1.126	0.134	3.724
7	0.042	0.207	0.211	0.188	0.054	0.494
8	0.042	0.075	0.076	0.072	0.032	0.146
9	0.042	0.098	0.099	0.096	0.056	0.161
3	0.021	0.059	0.062	0.058	0.029	0.112
4	0.021	0.084	0.085	0.081	0.040	0.154
5	0.021	0.208	0.207	0.196	0.045	0.425
6	0.021	0.598	0.627	0.551	0.065	1.852
7	0.021	0.103	0.105	0.094	0.029	0.246
8	0.021	0.037	0.038	0.036	0.015	0.072
9	0.021	0.049	0.050	0.048	0.027	0.081
3	0.008	0.023	0.023	0.022	0.011	0.043
4	0.008	0.032	0.033	0.031	0.015	0.058
5	0.008	0.079	0.079	0.075	0.018	0.164
6	0.008	0.228	0.243	0.212	0.024	0.713
7	0.008	0.039	0.040	0.036	0.010	0.097
8	0.008	0.014	0.015	0.014	0.006	0.028
9	0.008	0.019	0.019	0.018	0.010	0.032

Table 7 PCB Concentrations in Sediment Protective for Selected Levels of Common Carp Tissue Concentrations

	Tissue (mg/kg)	Data RAO	Bootstrap RAO Distribution (mg/kg)			
			Mean	Median	LCL95	UCL95
3	0.042	0.024	0.025	0.024	0.013	0.043
4	0.042	0.012	0.012	0.012	0.006	0.023
5	0.042	0.128	0.132	0.124	0.028	0.293
6	0.042	0.298	0.317	0.278	0.035	0.915
7	0.042	0.103	0.109	0.095	0.028	0.263
8	0.042	0.027	0.029	0.027	0.011	0.061
9	0.042	0.189	0.195	0.186	0.100	0.339
3	0.021	0.012	0.012	0.012	0.006	0.022
4	0.021	0.006	0.006	0.006	0.003	0.011
5	0.021	0.064	0.065	0.060	0.014	0.143
6	0.021	0.149	0.161	0.141	0.018	0.474
7	0.021	0.052	0.055	0.049	0.014	0.131
8	0.021	0.013	0.015	0.013	0.005	0.032
9	0.021	0.094	0.098	0.094	0.050	0.169
3	0.008	0.005	0.005	0.004	0.002	0.008
4	0.008	0.002	0.002	0.002	0.001	0.004
5	0.008	0.024	0.025	0.024	0.006	0.055
6	0.008	0.057	0.060	0.053	0.006	0.173
7	0.008	0.020	0.021	0.018	0.005	0.050
8	0.008	0.005	0.006	0.005	0.002	0.012
9	0.008	0.036	0.037	0.035	0.019	0.064